Executive Summary

IMPROVEMENT OF THE EMISSION INVENTORY FOR REACTIVE ORGANIC GASES AND OXIDES OF NITROGEN IN THE SOUTH COAST AIR BASIN

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This report was submitted in fulfillment of ARB Contract Number A2-076-32--Improvement of Emission Inventories for Reactive Organic Gases and Oxides of Nitrogen in the South Coast Air Basin, by Systems Applications, Inc. under the sponsorship of the California Air Resources Board. Work was completed as of 22 August 1984.

1 RESULTS AND CONCLUSIONS

This study was sponsored by the Air Resources Board (ARB) and performed by Systems Applications, Inc. and its subcontractor, Radian Corporation, to improve the quality of the 1979 California South Coast Air Basin (SOCAB) emission inventory. The primary motivation for the study involved improvement in the precision of emission estimates of reactive organic gases (ROG) and oxides of nitrogen (NO_x) for use in photochemical modeling activities. The study involved surveys, sampling activities, and laboratory analyses to develop information for updating the 1979 SOCAB inventory of ROG and NO_x emissions in the gridded Modeling Emission Data (MED) format. Section 2 of this summary provides an overview of study activities.

EMISSION DATA AND ORGANIC GASES

The major changes in emission data and classes of organic gases resulting from the inventory revisions are as follows:

(1) Overall total organic gas (TOG) and ROG emissions increased by 6.2 and 7.5 tons/day, respectively, and NO_x emissions decreased by 15.6 tons/day. This represents a change in stationary and off-road mobile source emissions in the inventory of 0.2, 1.0, and -3.0 percent for TOG, ROG, and NO_x emissions, respectively. These percentage changes are within the overall estimated variation for typical inventory emission totals. Thus, on the basis of this study, the 1979 total inventory of TOG and NO_x emissions was found to be a reasonably accurate representation of the actual basin-wide inventory. In addition, significant changes to both individual source and source category emissions and to ROG speciation were made during the study.

(2) Emissions of TOG and ROG for petroleum refining and marketing activities decreased. Although petroleum production TOG emissions increased, ROG emissions decreased as a result of a change in speciation. Emissions of TOG and ROG from certain categories of surface coating and solvent use increased.

(3) Petroleum refining NO_x emissions increased, whereas NO_x emissions from unspecified sources of fuel combustion decreased.

(4) Classes of organic gases: emissions of olefins and aromatics increased, and emissions of paraffins, carbonyls, and ethylene decreased. It is signficiant that the aromatic component of the overall inventory increased by 11.8 tons/day, primarily as a result of the improved speciation profiles for surface coating categories. At the same time, substantial decreases in the aromatic portion of emissions from petroleum refining and marketing categories were primarily the result of revised speciation profiles for gasoline. Thus, important inventory changes in organic gas reactivity have occurred as a result of this study.

(5) Other important changes not apparent through a review of emission totals were also made to the inventory. Revisions were incorporated into the MED file for the diurnal distribution of emissions from power plants, which comprise the largest stationary source category of NO_x emissions in the inventory. There were also changes to the spatial resolution of the inventory, particularly as a result of the redistribution of TOG emissions among sources of oil and gas production.

SPECIATION

The profiles used to speciate TOG emissions are the most uncertain component of a high-resolution inventory. Because of the need for accurate speciation data and the expectation that this need will increase in the future (particularly for photochemical modeling activities), the speciation profiles that currently exist fall considerably short of meeting this need. The primary source of speciation data is the EPA volatile organic compound (VOC) species data manual. This EPA document contains many species profiles for a variety of emission source categories, but is lacking in several respects.

(1) Many important source categories are not included in the manual.

(2) Some of the profiles are too limited to be useful. For example, profiles were developed for individual surface coating samples rather than for representative composite samples of a coating type (e.g., enamel, primer, lacquer, etc.).

(3) Some of the profiles are outdated. For instance, the composition of solvents used in surface coatings has changed significantly as a result of regulations regarding the organic content of coatings.

(4) The majority of the profiles are based on engineering evaluations and literature reviews employing limited data, rather than on direct sampling and analysis. As a result, many of the profiles are considered to be uncertain.

This study emphasized improvement in the state of knowledge for reactive species comprising TOG emissions from gasoline evaporative losses, coatings, and solvents. As a result, the speciation of both the overall inventory and several individual categories has been modified, particularly for aromatic organic gases. Furthermore, our new speciation profiles represent the first major update of the initial profile development for non-motor-vehicle sources performed by KVB in 1978. These new profiles are also expected to be used in the development of high-resolution inventories throughout the country. Thus, the work reported here has taken on nationwide significance.

UNCERTAINTIES

This research effort has improved the understanding of the primary types of uncertainties in high-resolution inventories and has reduced their extent in the 1979 SOCAB inventory. For example, it was found that

(1) Eight of the approximately 160 facilities surveyed in this study had been counted twice.

(2) Eight categories of sources, such as storage tank cleaning, were not accounted for by the 1979 inventory.

(3) A random error of about 27 tons/day of TOG emissions was found in the inventory.

(4) Systematic trends that either over- or underpredict emissions--such as a 2 tons/day increase in TOG emissions from surface coating and solvent usage facilities in the survey--are present in the inventory.

RECOMMENDATIONS

Twelve recommendations for guiding future activities in the area of emission inventory development are presented in the report. The most significant of these are the following:

(1) We made significant revisions to species profiles for gasoline and different types of coatings. Additional development of TOG speciation profiles for other source categories not examined in this study will lead to further significant improvement in ROG inventories for California. Therefore, the study team recommends that future research programs continue to emphasize the improvement of organic gas speciation profiles. Much work needs to be done in examining and improving TOG species profiles primarily because there has been relatively little effort in this area during the last decade. It is a demanding task to set priorities regarding the source types most needing investigation because so many categories need in-depth evaluation. Furthermore, the level of effort that should be expended is considerable. In addition, we recommend that the new TOG profiles developed in this study be used to develop ROG estimates for source categories in other portions of the state.

(2) It is important to emphasize the need for an accurate categorization of emissions into source classification codes (SCCs). Since the development of the 1979 inventory, more attention is now being given to this activity by the South Coast Air Quality Management District (SCAQMD). We recommend continued emphasis on the use of the emission fee data to properly allocate emissions into SCCs because of the importance of SCCs in identifying emissions (including toxic air contaminants) by source type, in evaluating control measures, and in assigning appropriate speciation profiles. The creation of accurate speciation profile and SCC descriptors is also important because they form the basis for the assignment of profiles and SCCs.

(3) Since the development of the 1979 inventory, more investigation into questionable data obtained from the data base has occurred at ARB and SCAQMD. Continued emphasis on matching emission fee data to emissions in the EIS file is recommended. We also recommend consideration of a single numbering system for all point sources in the SOCAB, which is under analysis at ARB and SCAQMD, in order to reduce the occurrence of double-counted sources.

(4) Particular attention should be given to improvements in the emission estimates for chemical manufacturing facilities. The existing TOG emission estimates were based on generalized emission factors in conjunction with total plant throughput. More specific estimates should be developed to improve the accuracy and level of detail of these estimates.

IMPLICATIONS OF THIS WORK

This study is a part of efforts by the state of California to improve and update its emission inventories. The implications of our work for ARB regulatory programs include the following study findings.

(1) Improvements to emission inventories for the state remain to be made; significant improvement is possible for high-resolution inventories.

(2) Poor speciation data are currently relied upon; these data should be improved because of their importance to ozone modeling studies and to the identification and quantification of toxic air contaminants.

(3) Revisions made in this study to speciation data may be of significance in interpreting the results of previous studies used to identify levels of source control for organic gases.

(4) Uncertainties existing in current inventories can be reduced through detailed evaluations.

2 OVERVIEW OF STUDY TASKS

This report summarizes a major study performed by Systems Applications and Radian Corporation to improve the quality of emission estimates and associated characteristics (e.g., spatial location and speciation profiles) of the 1979 gridded SOCAB emission inventory. The primary motivation for the study involved improvement in the emission estimates of ROG and NO_x to better reflect actual emissions of organic gases and NO_x for use in modeling photochemically reactive pollutants.

Over the years, various agencies have sponsored many studies to improve emission inventories and data bases, particularly for the SOCAB. The fundamental purposes of such work have been (1) to improve the understanding of sources and their emissions and (2) to assist modeling efforts aimed at establishing air quality impacts, appropriate control strategies, and permit conditions. Throughout this work, concerns have arisen that due to uncertainties, emission inventories may not reflect actual emission levels into the atmosphere. Our study sought to improve the SOCAB inventory and, where possible, to enhance all ROG and NO_x inventories in the state (e.g., through better speciation data).

Since the primary purpose of the study was to improve the original SOCAB inventory for use in high-resolution (i.e., detailed spatial and temporal specification) photochemical modeling activities, emphasis was given to reducing uncertainty in ROG emissions. We examined ROG and NO_x emissions from both point and area stationary sources and developed four major tasks for upgrading the MED inventory:

(1) A review of inventory data and photochemical modeling results to identify those source categories most likely to cause uncertainty in predicted ozone concentrations.

(2) A survey of selected sources in southern California to provide basic information for upgrading emission estimates, operating schedules, source identifications, etc.

(3) A test program for gathering improved data on organic gas speciation.

(4) The development of an improved ROG and NO_x inventory for the SOCAB compatible with the MED inventory format.

The main report for this study is composed of two volumes including eight detailed appendixes. The primary study product is a revised set of computer files representing the MED inventory. To generate the upgraded set of MED files, a substantial body of data and information was developed during the project. Much of this information will also be useful to the state and local control agencies in improving the data bases from which the original inventory was derived.

THE 1979 SOCAB INVENTORY

The overall study objectives were to uncover uncertainties and errors in the inventory, and to reduce or eliminate them to improve the quality of the inventory. The original 1979 SOCAB inventory was received in June 1983 and included computerized data files in MED format for TOG, NO_x, carbon monoxide, and sulfur oxide emissions. There are seven MED files of emission data, organic gas speciation information, and stack data. The emission data are divided into point source and area source files. The inventory provides hourly emission rates for a summer weekday in 1979 and consists of 5-kilometer-square grid cells for the SOCAB.

Table 2-1 presents 1979 SOCAB emission totals in the old inventory category (OIC) format as received from the ARB. Note that on-road motor vehicle emissions, which were not examined during this project, are excluded from this table. Thus, "total emissions" in the table do not reflect the sum of emissions from all categories of sources in the region. This convention of reporting emissions only for stationary and off-road mobile sources is consistent with the project's focus and is followed throughout the report. Emissions of TOG and ROG are expressed in the report by weight equivalent of methane, and NO_x and SO_x emissions are expressed by weight equivalent of nitrogen dioxide and sulfur dioxide, respectively.

TASK 1: IDENTIFICATION OF SOURCE CATEGORIES FOR FURTHER STUDY

The first task involved the identification of those source categories that cause the largest potential uncertainty in downwind ozone predictions. To identify these categories, the inventory was examined to determine the relative contribution of different components to inventory uncertainty. Information thus obtained was used to rank the source categories on the

TABLE 2-1. Original emission data by OIC code.

(Tons per day)

CODE	SOURCE	NAME	TOG	ROG	CO	NOX	SOX
100	FUEL COMBUSTION		0.00	0.00	0.00	0.00	0.00
110		AGRICULTURAL	0.00	0.00	0.00	0.03	0.00
120		OIL AND GAS PRODUCTION	3.79	0.66	1.07	7.48	0.10
130		PETROLEUM REFINING	11.05	4.67	3.68	59.35	6.21
140		OTHER MANUFACTURING/INDUSTRIAL	7.35	3.03	71.13	62.41	16.04
150		ELECTRIC UTILITIES	12.03	8.41	14.21	136.36	89.38
160		OTHER SERVICES AND COMMERCE	3.75	0.82	2.07	25.25	1.64
170		RESIDENTIAL	1.84	0.67	1.75	27.30	0.05
199		OTHER	15.78	2.11	12.73	43.92	0.66
200	WASTE BURNING		0.00	0.00	0.00	0.00	0.00
210		AGRICULTURAL DEBRIS	0.06	0.02	0.76	0.00	0.00
220		RANGE MANAGEMENT	0.00	0.00	0.00	0.00	0.00
230		FOREST MANAGEMENT	0.00	0.00	0.00	0.00	0.00
240		INCINERATION	0.16	0.04	0.43	0.42	3.39
299		OTHER	0.00	0.00	0.34	0.00	0.00
300	SOLVENT USE		0.00	0.00	0.00	0.00	0.00
310		DRY CLEANING	11.60	8.20	0.00	0.00	0.00
320		DEGREASING	33.94	23.15	0.00	0.13	0.00
330		ARCHITECTURAL COATING	88.91	87.98	0.00	0.00	0.00
340		OTHER SURFACE COATING	141.40	138.71	0.38	0.39	0.04
350		ASPHALT PAVING	32.28	22.83	0.00	0.00	0.00
360		PRINTING	12.40	12.04	0.01	0.13	0.00
370		DOMESTIC	46.26	39.63	0.00	0.00	0.00
380		INDUSTRIAL SOLVENT USE	23.16	22.64	0.00	0.02	0.00
399		OTHER	2.03	1.88	0.00	0.00	0.00
400	PETROLEUM PROCESS, STORAGE & TRANSFER		0.00	0.00	0.00	0.00	0.00
410		OIL AND GAS EXTRACTION	56.86	40.45	0.00	0.11	0.00
420		PETROLEUM REFINING	55.51	49.13	15.82	13.30	56.81
430		PETROLEUM MARKETING	372.18	84.02	0.00	0.03	0.00
499		OTHER	12.43	10.04	0.02	0.08	0.00
500	INDUSTRIAL PROCESSES		0.00	0.00	0.00	0.00	0.00
510		CHEMICAL	10.60	7.89	2.57	0.50	2.16
520		FOOD AND AGRICULTURAL	10.03	8.28	0.25	0.35	0.02
560		MINERAL PROCESSES	1.11	0.75	6.97	4.27	3.10
570		METAL PROCESSES	4.31	2.26	164.61	5.64	10.90
580		WOOD AND PAPER	0.13	0.09	0.00	0.07	0.00
599		OTHER	4.11	3.08	0.01	0.49	0.03
600	MISC PROCESSES		0.00	0.00	0.00	0.00	0.00
610		PESTICIDE APPLICATION	15.34	13.07	0.00	0.00	0.00
620		FARMING OPERATIONS	137.34	15.73	0.00	0.00	0.00
630		CONSTRUCTION AND DEMOLITION	0.00	0.00	0.00	0.00	0.00
640		ENTRAINED ROAD DUST - PAVED	0.00	0.00	0.00	0.00	0.00
650		ENTRAINED ROAD DUST - UNPAVED	0.00	0.00	0.00	0.00	0.00
660		UNPLANNED FIRES	85.95	47.77	499.94	10.77	0.00
680		SOLID WASTE LANDFILL	1638.83	18.16	0.00	0.00	0.00
699		OTHER	13.31	9.42	0.13	0.67	0.09
700	ON ROAD VEHICLES		0.00	0.00	0.00	0.00	0.00
710		LIGHT DUTY PASSENGER	0.00	0.00	0.00	0.03	0.00
720		LIGHT AND MEDIUM DUTY TRUCKS	0.00	0.00	0.00	0.03	0.00
730		HEAVY DUTY GAS TRUCKS	0.00	0.00	0.00	0.03	0.00

TABLE 2-1 (concluded)

CODE	SOURCE NAME	TOG	ROG	CO	NOX	SOX
740	HEAVY DUTY DIESEL TRUCKS	0.00	0.00	0.00	0.00	0.00
750	MOTORCYCLES	0.00	0.00	0.00	0.00	0.00
800	OTHER MOBILE	0.00	0.00	0.00	0.00	0.00
810	OFF ROAD VEHICLES	31.04	26.07	108.70	8.22	0.87
820	TRAINS	6.53	5.98	10.04	21.09	2.14
830	SHIPS	1.78	1.63	3.51	12.70	17.37
850	AIRCRAFT - GOVERNMENT	0.17	0.17	1.53	0.49	0.07
860	AIRCRAFT - OTHER	19.56	18.94	83.79	11.99	1.12
870	MOBILE EQUIPMENT	24.07	19.56	160.87	73.27	5.36
880	UTILITY EQUIPMENT	12.42	10.39	110.97	1.66	0.05
900	UNSPECIFIED SOURCES	0.00	0.00	0.00	0.00	0.00
TOTAL		2962.42	771.98	1278.27	528.90	217.61

basis of their estimated contribution to uncertainty in downwind ozone predictions. This ranked list was further examined, and a subset was recommended for investigation during the remainder of the project.

The categorization scheme selected for Task 1 was based on the source classification code (SCC--point sources) and the category of emission source (CES--area sources) systems employed in the 1979 data base. Task 1 was delineated into three steps. In Step 1, SCC and CES categories were ranked on the basis of their ROG emission levels and hydroxyl reactivity. Six source characteristics were then used in Step 2 to rerank the categories. The uncertainty and variability in the following six characteristics were evaluated:

Speciation profiles
Emission factors
Activity (throughput) data
Control effectiveness
Temporal distributions
Effect of stack height on ozone model predictions

These rankings were carefully scrutinized in Step 3 to formulate the final Task 1 list of categories recommended for further investigation. The improvements made to the emission inventory through survey and testing of these categories accomplished the study objective of reducing uncertainty in specific emission estimates.

Table 2-2 identifies the general source types selected from both the point and area source files that the study team recommended for detailed examination. Specific SCCs and CESs for the categories of point and area sources given in Table 2-2 formed the basis of the remainder of the study.

<u>Use of Task 1 Results in Other Studies</u>

The categories listed in Table 2-2 represent a fraction of the total number of categories in the inventory. An additional benefit resulting from this study is that the methodology created to rank all source categories in the inventory provides valuable guidance for further studies. Most important, hundreds of SCCs and CESs have now been examined and ranked for emission inventory uncertainties. These rankings can thus be used to establish priorities during the conception and performance of future studies aimed at improving the quality of ROG and NO_x emission inventories.

TABLE 2-2. Categories of sources recommended for further investigation.

Point Source File	Area Source File
Power plants--temporal data	Asphalt paving
Refineries	Stationary internal combustion engines
Bulk plants and terminals	Gasoline evaporation at service stations
Surface coating facilities	Unspecified emissions
Storage tanks	
Oil and gas production	
Chemical manufacturing	

TABLE 2-3. Types of facilities selected for the survey.

Type of Facility	No. of Facilities
Facilities from EIS File	
Surface coating	36
Refinery	14
Chemical plant	6
Petroleum bulk plant/terminal	5
Tire manufacturing	2
Fuel oil pumping	2
Oil production	1
Power plant	1
Lube oil blending	1
Facilities from EDP File	
Surface coating	57
Petroleum bulk plant/terminal	11
Oil production	6
Chemical plant	6
Chemical bulk plant/terminal	5
Surface coating manufacturing	4
Gas processing or compression plant	3
Oil industry research laboratory	1

TASK 2: SURVEY AND INVESTIGATION OF SELECTED SOURCE CATEGORIES

Survey Procedures

After identifying the source types recommended for further study, the next task involved a survey of facilities in the SOCAB representative of these source types. For point sources, this process involved a random selection of grid cells, followed by a random selection of facilities for the SCCs selected in Task 1. For area sources, "individual facilities" were not listed in the inventory since, by definition, each CES is a group of sources distributed throughout the SOCAB. Therefore, we examined the methods used to generate the emission estimates for particular area sources including, for example, a review of emission factors, activity (throughput) data, speciation profiles, etc.

The individual facilities to be surveyed were randomly chosen in a manner consistent with the selection procedure. Data from the Emission Data System (EDS) were then obtained from the ARB in the form of turnaround documents (TADs) for each of the selected facilities to assist in the survey formulation. A total of 161 facilities were selected for survey, which included all source categories of interest. Facilities selected from the Emission Inventory System (EIS) and Electronic Data Processing (EDP) files are categorized in Table 2-3. After comparing emission fee data with inventory information for a number of facilities, it was decided that each process at most facilities would be investigated. This resulted in a greatly increased project effort.

Two sets of questionnaires, an introduction, and a cover letter were developed for use in the survey. The first set of questionnaires was designed to investigate emission sources currently included in the inventory as well as all emission sources that should have been included. The second set of questionnaires was designed to investigate source categories possibly missing from the inventory. Efforts were first directed toward an initial contact of facility operators and then toward extensive follow-up to obtain survey responses. As a result, a 90 percent survey response was achieved, which is considered to be quite high. This high survey response appears to be the result of the following survey procedures:

(1) The initial facility contact to identify a responsible individual prior to sending the survey.

(2) The use of a cover letter on ARB letterhead.

(3) The comprehensive survey follow-up.

Investigation of Systematic Errors and Weaknesses in the Inventory

The approach used to address systematic errors in the inventory consisted of three types of activities: (1) survey and investigation of selected facilities, (2) investigation of selected source categories, and (3) review of species profile development and assignment. The survey and investigation of selected facilities was designed to address weak areas in the inventory such as the breakdown of emissions by SCC and the emission estimates from storage tanks. The investigation of selected facilities also included missing source categories (e.g., storage tank cleaning and industrial solvents) and double counting of sources. The second activity involved an investigation of selected source categories, including stationary internal combustion engines, oil and gas production, and power plant operating characteristics. Finally, the speciation of TOG emissions was reviewed and is described subsequently.

Examination of Selected Source Categories

Three source categories were selected for in-depth investigation in addition to the survey of facilities:

(1) Power plants--Information on the temporal distribution of power plant emissions in the SOCAB was obtained and evaluated to develop a diurnal operating profile.

(2) Stationary reciprocating internal combustion engines--Emissions were reallocated from the area source file to the point source file to improve the accuracy and spatial distribution of the emission estimates.

(3) Oil and gas production--The existing fugitive TOG emission estimates, which were based on an emission factor and the production rate for each field, were replaced by emission estimates from a recent ARB study. For oil and gas fields with large emission rates, detailed estimates were entered into the inventory by source category. For other fields, a single emission estimate for each field was entered.

TASK 3: SPECIES PROFILE DEVELOPMENT

The profiles used to speciate TOG emissions, which identify individual organic compounds and their weight percents, are considered the most uncertain component of the inventory. Accordingly, two methods were used in this study to develop improved organic gas species profiles: (1) sampling and analysis techniques and (2) a review of existing data. Table 2-4 lists the 68 profiles we developed from both test results and existing information.

Profiles Developed Through Analytical Work

At the beginning of this task, two general types of source testing and analysis were considered--one directed at improving emission estimates and one directed at improving speciation. After studying the options, it was concluded that all testing should be directed toward improving speciation. The source categories selected for testing are summarized in this section.

An integral part of the speciation test program was the determination of the composition of the samples to be analyzed as well as the specification of the analytical protocols. During the program, plans for the sampling and analysis activities were reviewed with several knowledgeable individuals, such as ARB chemists, particularly regarding test procedures considered to be nonstandard.

Gasoline

Analyses were performed on liquid and static vapor samples from four product types of winter- and summer-blend gasolines. Using the results from a total of 18 gasoline analyses, 22 liquid and vapor profiles were developed. The compositions of liquid and static vapor profiles were found to differ considerably. The paraffin content of static vapor samples was found to be much higher than that of liquid samples. Furthermore, the unleaded liquid samples tended to have a higher aromatic content than did the leaded liquid samples.

The comprehensive analyses performed for gasoline samples represent more extensive results than originally called for by the scope of the project. Profiles of liquid gasoline are now available for evaporative losses resulting from such occurrences as gasoline spillage. Similarly, related gasoline profiles for static vapor emissions are available for such conditions as storage tank losses.

Industrial Surface Coatings

Composite profiles for industrial surface coating samples were developed by focusing on four coating types: lacquer, enamel, primer, and adhesive. Efforts were made to obtain representative samples of these

TABLE 2-4. New profiles developed in this study.

Profile Code	Profile Description
701	LIQUID GASOLINE - UNLEADED REGULAR - SUMMER BLEND
702	LIQUID GASOLINE - LEADED REGULAR - SUMMER BLEND
703	LIQUID GASOLINE - UNLEADED PREMIUM - SUMMER BLEND
704	LIQUID GASOLINE - LEADED PREMIUM - SUMMER BLEND
705	GASOLINE VAPORS - UNLEADED REGULAR - SUMMER BLEND
706	GASOLINE VAPORS - LEADED REGULAR - SUMMER BLEND
707	GASOLINE VAPORS - UNLEADED PREMIUM - SUMMER BLEND
708	GASOLINE VAPORS - LEADED PREMIUM - SUMMER BLEND
709	LIQUID GASOLINE - COMPOSITE OF PRODUCT - SUMMER BLEND
710	GASOLINE VAPORS - COMPOSITE OF PRODUCT - SUMMER BLEND
711	INDUSTRIAL SURFACE COATING - COMPOSITE LACQUER
712	INDUSTRIAL SURFACE COATING - COMPOSITE ENAMEL
713	INDUSTRIAL SURFACE COATING - COMPOSITE PRIMER
714	INDUSTRIAL SURFACE COATING - COMPOSITE ADHESIVE
715	SLOW CURE ASPHALT
716	MEDIUM CURE ASPHALT
717	ARCHITECTURAL SURFACE COATING - WATER BASED PAINT
718	ARCHITECTURAL SURFACE COATING - COMPOSITE SOLVENT
719	INTERNAL COMBUSTION ENGINE - RECIPROCATING-NATURAL GAS FIRED
721	LIQUID GASOLINE - UNLEADED REGULAR - WINTER BLEND
722	LIQUID GASOLINE - LEADED REGULAR - WINTER BLEND
723	LIQUID GASOLINE - UNLEADED PREMIUM - WINTER BLEND
724	LIQUID GASOLINE - LEADED PREMIUM - WINTER BLEND
725	GASOLINE VAPORS - UNLEADED REGULAR - WINTER BLEND
726	GASOLINE VAPORS - LEADED REGULAR - WINTER BLEND
727	GASOLINE VAPORS - UNLEADED PREMIUM - WINTER BLEND
728	GASOLINE VAPORS - LEADED PREMIUM - WINTER BLEND
729	LIQUID GASOLINE - COMPOSITE OF PRODUCT - WINTER BLEND
730	GASOLINE VAPORS - COMPOSITE OF PRODUCT - WINTER BLEND
731	HEATED GASOLINE VAPORS - UNLEADED REGULAR - SUMMER BLEND
732	AGITATED GASOLINE VAPORS - UNLEADED REGULAR - SUMMER BLEND
751	ACRYLONITRILE-BUTADIENE-STYRENE (ABS) RESIN MFG.
752	POLYSTYRENE RESIN MFG.
753	STYRENE
754	CHLOROSOLVE
755	TRICHLOROTRIFLOUROETHANE
756	OIL AND GAS PRODUCTION FUGITIVES-LIQUID SERVICE
757	OIL AND GAS PRODUCTION FUGITIVES-GAS SERVICE
758	OIL AND GAS PRODUCTION FUGITIVES-VALVES-UNSPECIFIED SERVICE
759	OIL AND GAS PRODUCTION FUGITIVES-FITTINGS-UNSPECIFIED SERVICE
760	EVAPORATIVE EMISSIONS-DISTILLATE FUEL
761	EVAPORATIVE EMISSIONS-NAPHTHA
762	BTX (BENZENE/TOLUENE/XYLENE)
763	PHTHALIC ANHYDRIDE MFG - XYLENE OXIDATION
764	FLUOROCARBON - 12/11 MANUFACTURING
765	FLUOROCARBON - 23/22 MANUFACTURING
766	FLUOROCARBON - 113/114 MANUFACTURING
767	FLUOROCARBON - 11

TABLE 2-4 (concluded)

Profile Code	Profile Description
768	FLUOROCARBON - 113
769	FLUOROCARBON - 114
770	CHLOROFLUOROCARBONS
771	CARBON TETRACHLORIDE
772	ORTHO-XYLENE
773	FLUOROCARBON MFG - VALVES, PUMPS, ETC
774	ISOBUTYL ACETATE
775	ISOBUTYL ALCOHOL
776	ISOBUTYL ISOBUTYRATE
777	METHYL AMYL KETONE
778	METHYL ISOBUTYL KETONE
779	N-BUTYL ACETATE
780	N-PROPYL ACETATE
781	N-PROPYL ALCOHOL
782	HEXYLENE GLYCOL
783	INDUSTRIAL SURFACE COATING - SOLVENT BASED PAINT
784	SYNTHETIC RUBBER MFG - STYRENE-BUTADIENE RUBBER
785	ETHYLENE OXIDE
786	METHYL ALCOHOL
787	CARBON BLACK MANUFACTURING

coating types from both industrial surface coating facilities and industrial surface coating manufacturers. We found that the new species profiles developed for each of the coating types have a high aromatic content, especially of toluene and xylene. This is in contrast to the currently used profiles, which consist primarily of "mineral spirits"--generally a mixture of C_6 to C_{10} straight-chain paraffins.

Asphalts--Slow Cure and Medium Cure

An extensive investigation of the composition of different asphalts was conducted during the study. One sample of slow-cure and one sample of medium-cure asphalt from the two refineries in the SOCAB that produce cutback asphalts were analyzed. Composite samples were developed by combining equal amounts of the asphalts from the two refineries. After the samples were analyzed and the profiles were developed, it was discovered that one of the individual samples used in each composite sample had been purposely altered by the supplier. We feel that the new profiles better represent emissions from cutback asphalts than does the current profile, but they merit further investigation.

Architectural Surface Coating--Water-Based Coatings

Using ARB statewide survey results for architectural surface coatings, four water-based product types were selected for composite testing: interior flats, exterior flats, interior nonflats, and exterior nonflats. Individual coatings were purchased at retail outlets and combined in proportion to their 1980 statewide sales to develop a composite sample. The composite sample was analyzed and the results were used to develop a new profile.

Architectural Surface Coating--Solvent Usage

Solvents were purchased from major retail paint outlets and combined into a composite sample on the basis of sales for the different solvents. Using the analytical results of the composite sample, a species profile was developed consisting of a variety of compounds with few halogenated hydrocarbons.

Internal Combustion Engines--Reciprocating-Natural Gas

Exhaust gas samples from two stationary natural-gas-fired internal combustion engines were obtained and analyzed for organic content including aldehydes. The primary constituent of the organic gases was methane, but other low molecular weight paraffins and olefins were also found.

Profiles Developed from Existing Data

In addition to developing species profiles through analytical work, profiles were developed through analyses of existing information. To develop new organic gas profiles from existing data, computerized literature and library searches were undertaken and information obtained in the survey of facilities was used. This major activity resulted in the generation of 37 new profiles. Furthermore, the speciation of TOG emissions in the inventory was also improved significantly through changes to SCCs used to identify emission sources and to assign speciation profiles.

In summary, important additions and revisions to several speciation profiles for organic gases resulted from the Task 3 sampling and analysis activities.

TASK 4: INVENTORY IMPROVEMENT

Procedures Used to Develop Changes to the 1979 Inventory

The existing inventory was first compared with information obtained from Task 2 survey responses and 1979 emission fee data. Recommended changes to the inventory were developed for specific point sources and were then incorporated into the MED files. A substantial body of data is contained in the detailed documentation for changes to the inventory.

During the development of inventory revisions, we generated 148 SCCs not available before this study. These new SCCs permitted a more specific identification of certain emission sources at the surveyed facilities and resulted in the assignment of more specific speciation profiles.

Results Obtained from Inventory Revisions

The emission changes affected facilties in all four counties of the SOCAB and included revisions primarily for TOG and NO_x emissions. Additions, deletions, and modifications to emission data were made for about 1500 MED entries for 241 facilities. Most of the emission changes to the MED file were on the order of 0.2 to 5.0 kilograms/hour, but changes as large as 150 kg/hr were also made. Eight cases of double counting of facilities were also uncovered and deleted from the MED file, as appropriate. Modifications to the MED files were incorporated for speciation profiles, which also resulted in the addition of many new organic species.

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Results obtained using the "old inventory category" (OIC) system for grouping sources are presented in Table 2-5 (the totals do not include on-road motor vehicle emissions). It was necessary to generate new OIC codes for reporting the revised emission totals. Although changes to the spatial and temporal resolution of the inventory cannot be ascertained from these revised emission totals, overall TOG and ROG emissions increased by 6.2 and 7.5 tons/day (0.2 and 1.0 percent), and NO_x emissions decreased by 15.6 tons/day (3.0 percent).

Important changes in the reactivity of organic gas emissions in the original and revised files were found to result from this study. Emissions for two of the five organic classes of pollutants--olefins and aromatics--increased and emissions for three classes--paraffins, carbonyls, and ethylene--decreased in the revised inventory. One of the most important effects of the modifications to the inventory is an increase of 11.8 tons/day in the aromatic component of the overall inventory. This is chiefly the result of the improved speciation profiles for surface coating categories; in particular, the aromatic portion of emissions from the category "other surface coating" increased more than 100 percent in the revised inventory. At the same time, substantial decreases in the aromatic portion of emissions from petroleum refining and marketing were primarily a result of revised profiles for gasoline. There is also a more reactive mix of organic gases overall in the revised inventory.

Inventory Uncertainties

Uncertainties in the emission inventory were found to be an important aspect of the study. We found significant systematic trends that either over- or underpredicted emissions in the inventory. In particular, emission estimates in the EDP file were generally made at the time that a permit was issued. Because permits have been issued over a number of years, emissions in the EDP file do not reflect 1979 conditions. For example, we analyzed the difference between the original emissions from the EDP file and the revised emissions calculated from the survey for surface coating and solvent usage facilities. The results showed the revised TOG emissions for these facilities to be almost four times higher than the corresponding values in the original inventory.

Errors of a random nature were also found in the inventory. The error of greatest significance affected the Yorba Linda oil field. The original TOG estimate of 27.1 tons/day for this oil field was revised to approximately one-tenth of its original value. It appeared that an error in an emission factor might have resulted from a transcription error. Further-

TABLE 2-5. Revised emission data by OIC code.

(Tons per day)

CODE	SOURCE NAME	TOG	ROG	CO	NOX	SOX
100	FUEL COMBUSTION	0.00	0.00	0.00	0.00	0.00
110	AGRICULTURAL	0.00	0.00	0.00	0.03	0.00
120	OIL AND GAS PRODUCTION	4.00	0.54	1.22	8.07	0.10
130	PETROLEUM REFINING	10.63	3.49	2.98	65.88	6.26
140	OTHER MANUFACTURING/INDUSTRIAL	7.41	3.03	71.15	63.62	16.15
150	ELECTRIC UTILITIES	13.49	0.37	14.77	137.00	89.38
160	OTHER SERVICES AND COMMERCE	3.74	0.80	2.07	25.80	1.63
170	RESIDENTIAL	1.84	0.67	1.75	27.30	0.05
199	OTHER	7.54	1.15	9.35	17.29	0.66
200	WASTE BURNING	0.00	0.00	0.00	0.00	0.00
210	AGRICULTURAL DEBRIS	0.06	0.02	0.76	0.00	0.00
220	RANGE MANAGEMENT	0.00	0.00	0.00	0.00	0.00
230	FOREST MANAGEMENT	0.00	0.00	0.00	0.00	0.00
240	INCINERATION	0.16	0.04	0.43	0.41	3.39
299	OTHER	0.00	0.00	0.34	0.00	0.00
300	SOLVENT USE	0.00	0.00	0.00	0.00	0.00
310	DRY CLEANING	11.60	8.20	0.00	0.00	0.00
320	DEGREASING	34.87	23.55	0.00	0.13	0.00
330	ARCHITECTURAL COATING	93.46	89.58	0.00	0.00	0.00
340	OTHER SURFACE COATING	153.93	151.19	0.39	0.39	0.04
350	ASPHALT PAVING	33.70	32.21	0.00	0.00	0.00
360	PRINTING	12.40	12.04	0.01	0.13	0.00
370	DOMESTIC	46.26	39.63	0.00	0.00	0.00
380	INDUSTRIAL SOLVENT USE	29.07	28.37	0.00	0.17	0.00
399	OTHER	1.85	1.77	0.00	0.00	0.00
400	PETROLEUM PROCESS, STORAGE & TRANSFER	0.00	0.00	0.00	0.00	0.00
410	OIL AND GAS EXTRACTION	66.91	36.86	0.00	0.03	0.00
420	PETROLEUM REFINING	48.70	42.58	16.17	13.10	54.56
430	PETROLEUM MARKETING	367.40	79.62	0.00	0.03	0.00
499	OTHER	9.06	7.89	0.02	0.08	0.00
500	INDUSTRIAL PROCESSES	0.00	0.00	0.00	0.00	0.00
510	CHEMICAL	6.61	5.53	2.55	0.48	2.16
520	FOOD AND AGRICULTURAL	9.98	0.24	0.25	0.35	0.02
560	MINERAL PROCESSES	1.11	0.75	6.97	4.27	3.10
570	METAL PROCESSES	4.25	2.22	164.61	5.64	10.90
580	WOOD AND PAPER	0.13	0.09	0.00	0.07	0.00
599	OTHER	4.81	4.61	0.01	0.45	0.03
600	MISC PROCESSES	0.00	0.00	0.00	0.00	0.00
610	PESTICIDE APPLICATION	15.34	13.07	0.00	0.00	0.00
620	FARMING OPERATIONS	137.34	15.73	0.00	0.00	0.00
630	CONSTRUCTION AND DEMOLITION	0.00	0.00	0.00	0.00	0.00
640	ENTRAINED ROAD DUST - PAVED	0.00	0.00	0.00	0.00	0.00
650	ENTRAINED ROAD DUST - UNPAVED	0.00	0.00	0.00	0.00	0.00
660	UNPLANNED FIRES	86.95	47.77	499.94	10.77	0.00
680	SOLID WASTE LANDFILL	1630.83	18.16	0.00	0.00	0.00
699	OTHER	12.64	8.94	0.13	0.67	0.09
700	ON ROAD VEHICLES	0.00	0.00	0.00	0.00	0.00
710	LIGHT DUTY PASSENGER	0.00	0.00	0.00	0.00	0.00
720	LIGHT AND MEDIUM DUTY TRUCKS	0.00	0.00	0.00	0.00	0.00
730	HEAVY DUTY GAS TRUCKS	0.00	0.00	0.00	0.00	0.00

TABLE 2-5 (concluded)

CODE	SOURCE	NAME	TOG	ROG	CO	NOX	SOX
740		HEAVY DUTY DIESEL TRUCKS	0.00	0.00	0.00	0.00	0.00
750		MOTORCYCLES	0.00	0.00	0.00	0.50	0.00
800	OTHER MOBILE		0.00	0.00	0.00	0.30	0.00
810		OFF ROAD VEHICLES	31.04	26.07	100.70	8.22	0.07
820		TRAINS	6.53	5.98	10.04	21.09	2.14
830		SHIPS	1.78	1.63	3.51	12.70	17.37
850		AIRCRAFT - GOVERNMENT	0.17	0.17	1.53	0.49	0.07
860		AIRCRAFT - OTHER	19.56	18.94	83.79	11.99	1.12
870		MOBILE EQUIPMENT	24.07	19.56	160.87	73.27	5.36
880		UTILITY EQUIPMENT	12.42	10.39	110.97	1.66	0.05
900	UNSPECIFIED SOURCES		0.00	0.00	0.00	0.20	0.00
TOTAL			2968.62	779.45	1275.28	513.29	215.50

more, the fact that eight cases of double-counted facilities were discovered during a survey of approximately 160 facilities is significant. We expect there are additional cases of double counting in the 1979 inventory. Uncertainties in the inventory also result from missing source categories, such as storage tank cleaning and petroleum vacuum trucks, and from operating deviations such as equipment upsets.

The collective experience of the project team with TOG, ROG, and NO_x inventories for the state, and in particular for the SOCAB, suggests that the uncertainty in the overall 1979 SOCAB inventory is in the range of 20 to 30 percent. This estimate is generally consistent with similar findings presented by several other inventory specialists.